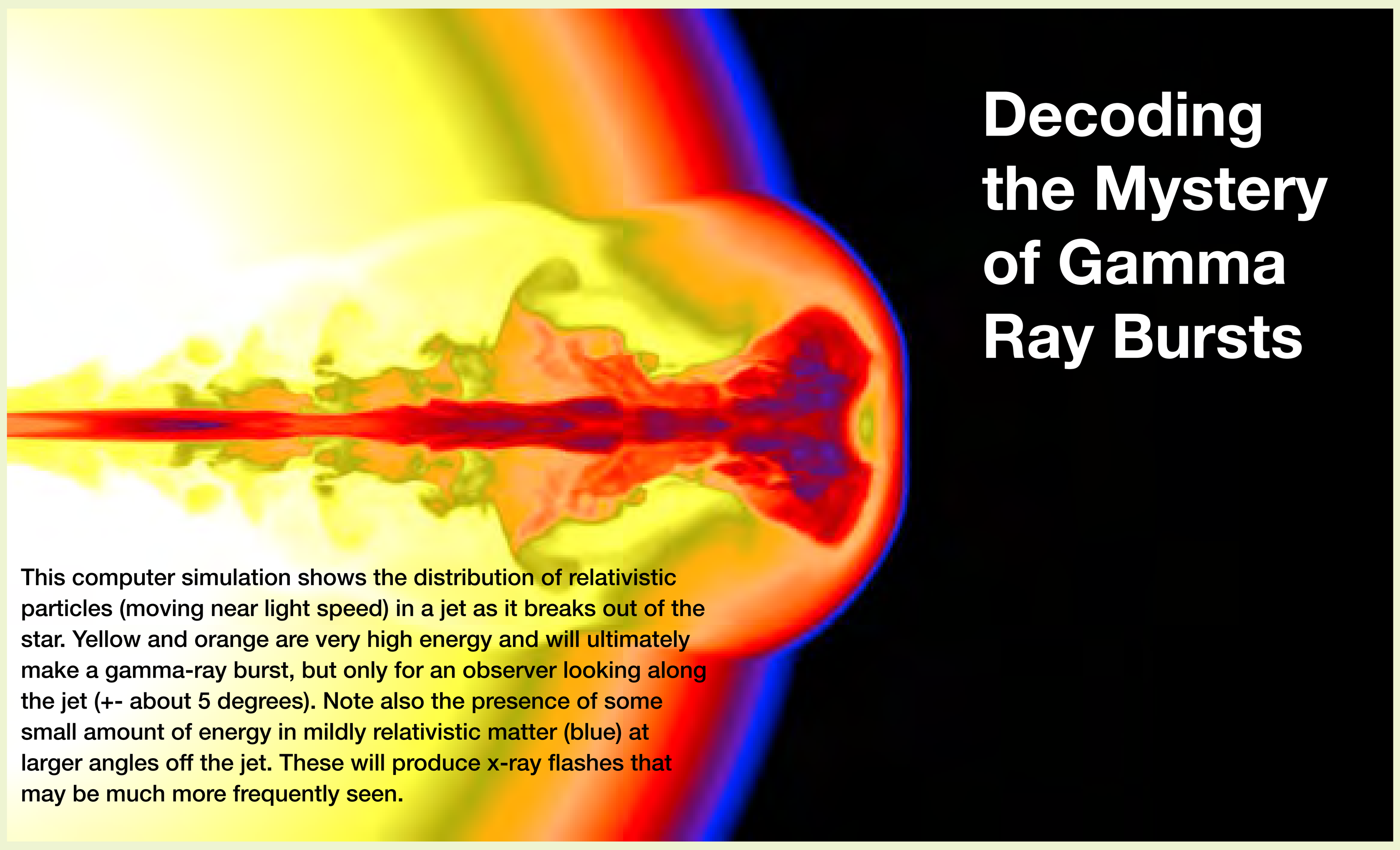
SCIENTIFIC COMPUTING LEADERSHIP

NERSC: ACCELERATING SCIENTIFIC DISCOVERY



This computer simulation shows the distribution of relativistic particles (moving near light speed) in a jet as it breaks out of the star. Yellow and orange are very high energy and will ultimately make a gamma-ray burst, but only for an observer looking along the jet (+- about 5 degrees). Note also the presence of some small amount of energy in mildly relativistic matter (blue) at larger angles off the jet. These will produce x-ray flashes that may be much more frequently seen.

The Propagation and Eruption of Relativistic Jets from the Stellar Progenitors of GRBs

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and A. Heger, Los Alamos National Laboratory

Astrophysical Journal, 608, 365, June 10, 2004

Scientists have pieced together the key elements of a gamma-ray burst, from star death to dramatic black hole birth, thanks to a March 29, 2003 explosion considered the "Rosetta stone" of such bursts. The findings support the collapsar model, where the core of a massive star collapses into a black hole. The black hole's spin or magnetic fields may be acting like a giant cosmic cannon shooting out many earth masses of matter at 99.999 per cent the speed of light. Scientists calculated that GRB030329 originated from a star at least 15 times more massive than the Earth's sun.

New two- and three-dimensional calculations on NERSC's IBM SP, Seaborg, show the break-out of so called "relativistic jets" as they erupt from the surface of the parent star. As it erupts, the jet's core is surrounded by a "cocoon" of less energetic, but still moderately relativistic ejecta that expands and becomes visible at larger polar angles. These less energetic ejecta may be the origin of X-ray flashes and other high-energy transients which will be visible to a larger fraction of the sky, albeit to a shorter distance than common gamma-ray bursts. Jet stability was also examined in three-dimensional calculations. If the jet changes angle by more than three degrees in several seconds, it will dissipate, producing a broad beam with inadequate Lorentz factor to make a common gamma-ray burst. This may be an alternate way to make X-ray flashes.

Study of Pentaquarks on the Lattice with Overlap Fermions

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Since the reported discovery two years ago of an exotic 5-quark resonance, named $\theta^+(uudd\bar{s})$, with a mass of about 1540 MeV and a narrow width of less than 20 MeV, there has been a rapid growth of interest in the subject. Eleven more experiments have reported the observation of the state. It also stimulated the search for other pentaquarks.

We present a quenched lattice QCD calculation of spin-1/2 five-quark states with $uudd\bar{s}$ quark content for both positive and negative parities. We do not observe any bound pentaquark state in these channels for either I = 0 or I = 1. The states we found are consistent with KN scattering states which are checked to exhibit the expected volume dependence of the spectral weight. The results are based on overlap-fermion propagators on two lattices, $12^3 \times 28$ and $16^3 \times 28$, with the same lattice spacing of 0.2 fm, and pion mass as low as 180 MeV.

Our results based on the overlap fermion with pion mass as low as 180 MeV seem to reveal no evidence for a pentaquark state of the type $uudd\bar{s}$ with the quantum numbers $I(J^P) = (0, 1)(1/2^{\pm})$ near a mass of 1540 MeV. Instead, the correlation functions are dominated by KN scattering states and the ghost KN_X states in the 1/2+ channel at low quark mass (pion mass less than 300 MeV). Our results are consistent with the known features of the KN scattering phase-shifts analysis. We have checked that the observed KN states exhibit the expected volume dependence in the spectral weight for two particles in a box. We advocate the use of this volume dependence to uncover the character of the states found in multi-quark calculations on the lattice. Our conclusion is in contradiction with the other lattice calculations which have claimed a pentaquark signal of either negative parity, or positive parity, in the vicinity of 1.54 GeV.

First Principles Methods Applied to Heterogeneous Catalysis

From resolving puzzles to identifying promising materials

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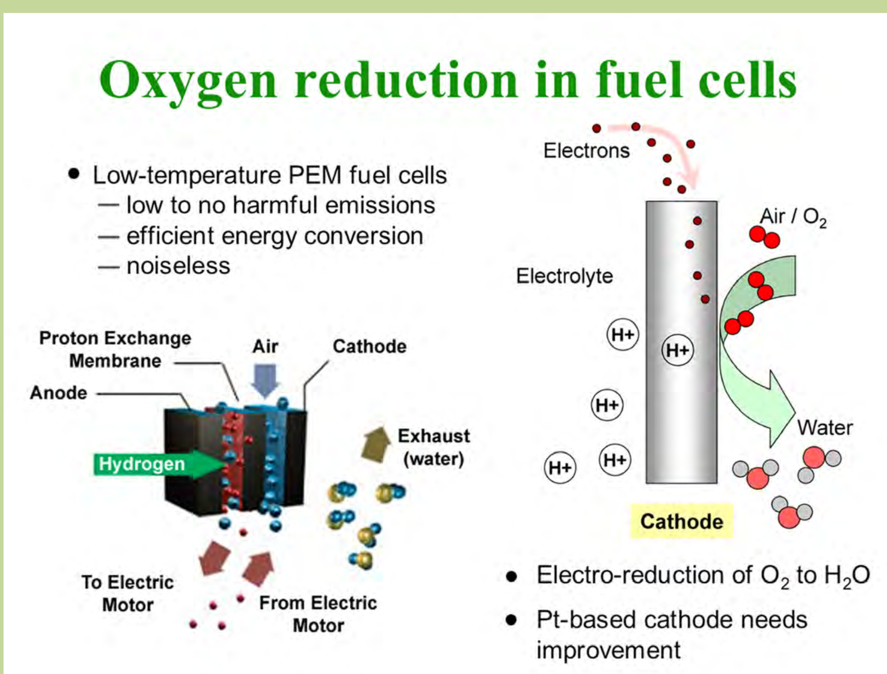
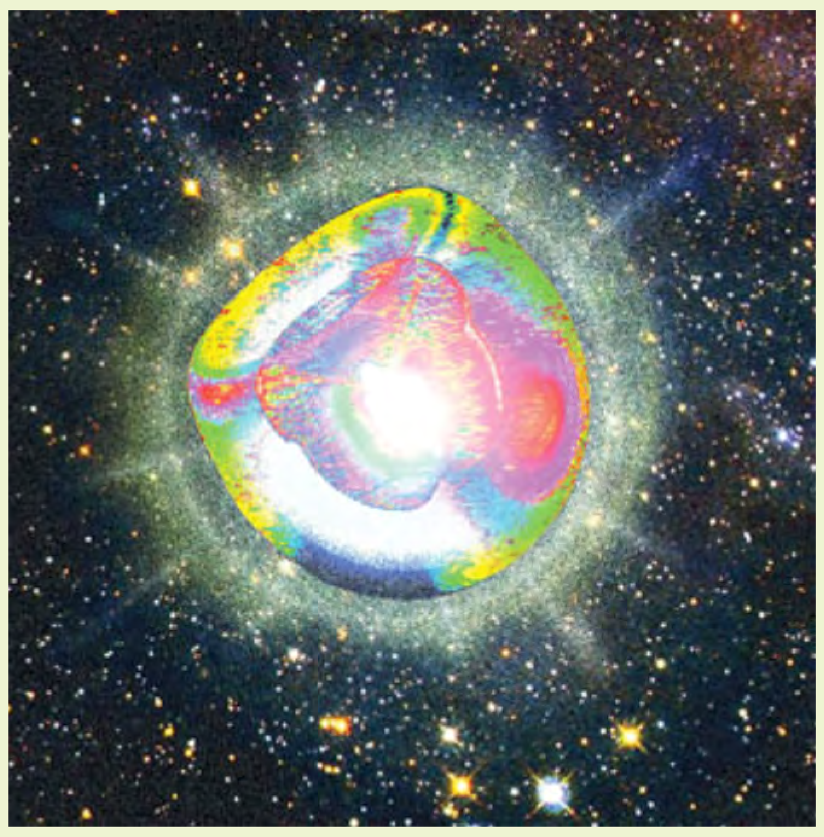
Low-temperature PEM fuel cells have low to no harmful emissions, efficient energy conversion, and are noiseless. In recent years, a number of platinum-base metal (Pt-M) alloys have been demonstrated to possess greater activity than pure Pt for catalyzing the oxygen reduction reaction (ORR) in acidic electrolytes, which is one of the primary electrochemical reactions in low-temperature fuel cells.

Self-consistent periodic density functional theory calculations have been performed to study the adsorption of O and O_2 and the dissociation of O_2 on the facets of ordered Pt_3Co and Pt_3Fe alloys and on monolayer Pt skins covering these two alloys.

We propose that an alleviation of poisoning by O and enhanced rates for reactions involving O may be some of the reasons why Pt skins are more active for the oxygen reduction reaction in low-temperature fuel cells.





Could There Be a Hole in Type Ia Supernovae?

Daniel Kasen, Peter Nugent, R. C. Thomas, and Lifan Wang, Lawrence Berkeley National Laboratory,

Astrophysical Journal, 610, 876, August 1, 2004

In the favored progenitor scenario, Type Ia supernovae (SNe Ia) arise from a white dwarf accreting material from a nondegenerate companion star. Soon after the white dwarf explodes, the ejected supernova material engulfs the companion star; two-dimensional hydrodynamic simulations by Marietta et al. (2000) show that in the interaction, the companion star carves out a conical hole of opening angle 30–40 degrees in the supernova ejecta.

In this paper associated with the poster we use multidimensional Monte Carlo radiative transfer calculations to explore the observable consequences of an ejecta-hole asymmetry. We calculate the variation of the spectrum, luminosity, and polarization with viewing angle for the aspherical supernova near maximum light. We find that the supernova looks normal from almost all viewing angles except when one looks almost directly down the hole. In the latter case, one sees into the deeper, hotter layers of ejecta. The supernova is relatively brighter and has a peculiar spectrum characterized by more highly ionized species, weaker absorption features, and lower absorption velocities. The spectrum viewed down the hole is comparable to those of the class of SN 1991T–like supernovae. We consider how the ejecta-hole asymmetry may explain the current spectropolarimetric observations of SNe Ia and suggest a few observational signatures of the geometry. Finally, we discuss the variety currently seen in observed SNe Ia and how an ejecta-hole asymmetry may fit in as one of several possible sources of diversity.

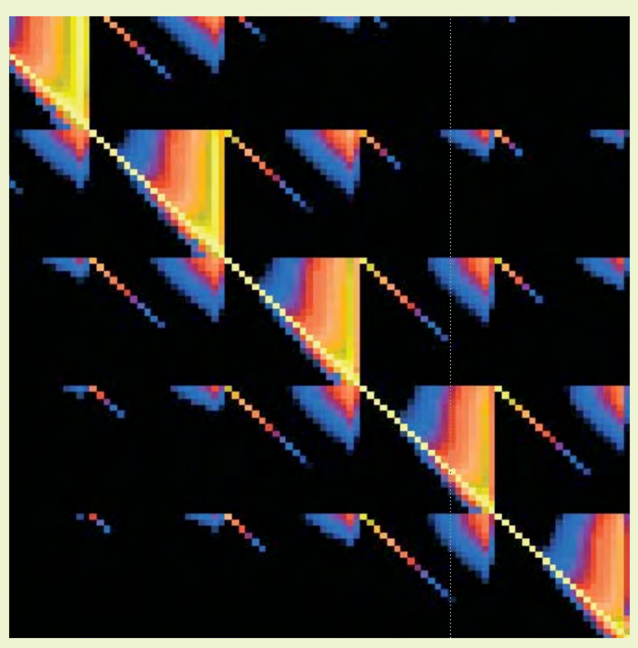
A Comparison of Algorithms for the Efficient Solution of the Linear Systems Arising from Multigroup Flux-Limited Diffusion Problems

F. Douglas Swesty, SUNY at Stony Brook; Dennis C. Smolarski, Santa Clara University; and Paul E. Saylor, University of Illinois at Champaign-Urbana

Astrophysical Journal Supplement Series, 153:369–387, 2004 July

One of the more challenging aspects of carrying out radiation-hydrodynamic models of core collapse supernovae on Terascale architectures is the parallelization of the implicit Multi-group flux-limited diffusion radiation transport algorithm. This algorithm requires the numerical solution of a large, sparse set of non-linear equations arising from the implicit finite-differencing of the underlying integro-partial differential equations.

The solution of these non-linear systems often dominates the computational cost of carrying out astrophysical simulations and efficient methods for solving these systems are highly desirable. The work carried out at NERSC uses Newton-Krylov iteration to solve these non-linear systems in a highly scalable fashion. This technique is accelerated through the use of sparse parallel approximate inverse preconditioners. These preconditioners exploit the known structure of the Jacobian operator to compute a very sparse approximate inverse operator whose elements are obtained via an embarrassingly parallel least-squares fit for every cell in the domain. The use of these preconditioners has accelerated the iterative performance of our radiation-transport models on NERSC's IBM SP, Seaborg.



False color image of the absolute value of the upper left (100 ; 100) corner of the inverse of the coefficient matrix for a test problem. Brighter colors indicate larger elements.

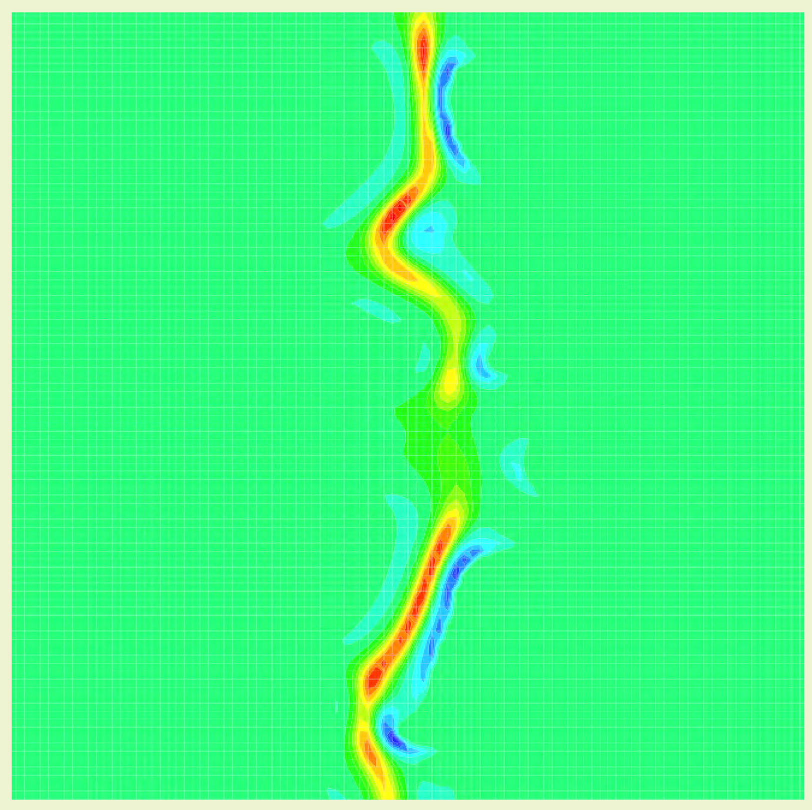
High-Fidelity Simulation of Turbulent Combustion with Detailed Chemistry

Hong G. Im, University of Michigan; Christopher J. Rutland, University of Wisconsin-Madison; Arnaud Trouve, University of Maryland; Jacqueline H. Chen, Sandia National Laboratories; Chunsang Yoo, University of Michigan; Yunliang Wang, University of Wisconsin-Madison; Yi Wang, University of Maryland; Evatt R. Hawkes, Sandia National Laboratories

Direct numerical simulation (DNS) is a mature and productive research tool in combustion science that is used to provide high-fidelity computer-based observations of the micro-physics found in turbulent reacting flows. Sponsored by DOE's program of "Scientific Discovery through Advanced Computing (SciDAC)," the scope of this project is to enhance the current DNS capability to the next level with new numerical and physical modeling capabilities. The project is a multi-institution, collaborative effort aimed at adapting S3D, a high-fidelity turbulent reacting flow solver, to terascale computer technology. Ultimately, the project is expected to enable first-principles simulations of pollutant emissions (NOx, soot) from turbulent combustion systems.

The capabilities of the new DNS code will be demonstrated by the simulation of compression-ignition of hydrocarbon fuels in a turbulent inhomogeneous mixture, and the simulation of NOx and soot emissions from hydrocarbon-air turbulent jet diffusion flames.

"Access to resources at NERSC has allowed large-scale computations to be performed, pushing the limits of combustion science," said Arnaud Trouve, a professor of engineering at the University of Maryland.



University of Michigan professor Hong Im and his team are working at NERSC to develop the physical modeling of soot formation and radiation processes. The image shows the generation of edge flames in a turbulent counterflow.

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